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Thermophysical properties of alkali halides

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Abstract : The thermophysical properties of alkali halides can be evaluated using their elastic constants which are obtained by ultrasonic techniques. The thermophysical properties are linearly dependent on the product of Debye temperature and square root of molecular weight. This dependency has been examined irrespective of *bcc* and *fcc* structure of alkali halides. In this work, a comparative study has been made between theoretical and experimental values of thermophysical properties of alkali halides.

Keywords : Elastic constants, debye temperature, coulomb force, thermal conductivity and melting temperature.

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In present days, considerable interest has been taken in the investigation of anharmonic, elastic and thermal properties of alkali halides [1,2]. These halides possess cubic crystal structure and compounds of alkali metals with halogen elements are also crystalline solids, which are of great interest for theoretical and experimental purposes. The Coulomb force binds the ions of alkali halides. Due to these factors, the alkali halides are relatively easy for theoretical and experimental studies.

The thermophysical lattice properties *viz.* Debye temperature (θ), melting temperature (T_m), thermal conductivity (K) and heat capacity (C) are derived by Kitaeva *et al* [3] using second order elastic constants data. These thermophysical properties are defined as:

Debye temperature

$$\theta = 251.40\left(\frac{d}{A}\right)^{\frac{1}{3}} V_m \qquad (1)$$

Melting temperature :

$$T_{m1} = C_1 V^2 V_m^{\frac{2}{3}} A\,,$$

$$T_{m2} = C_2 v_m^2 A\,, \qquad (2)$$

Thermal conductivity :

$$K = \frac{C_3 \xi A \delta \theta^3}{\gamma^2 T}\,, \qquad (3)$$

Heat capacity :

$$C_v = \frac{3R}{2A}\left\{\left[\frac{e^x X^2}{\left(e^x-1\right)^2}\right]+\left[\frac{e^{2x}(2X)^2}{\left(e^{2x}-1\right)^2}\right]\right\},$$

$$C_p = C_v + 0.0214 C_v^2 \frac{T}{T_m}\,, \qquad (4)$$

where

d = density, $X = \theta/2T$, V_m = molar volume, M = molecular weight, T = temperature, C_1, C_2 & C_3 = constants, A = M/p = atomic weight, R = gas constant, γ = Gruneisen constant, p = number of atoms, $V = \theta h/k$ = characteristic frequency, v_m = mean acoustic velocity, δ = mean volume = $a^3/16$ ('a' is lattice constants), C_p & Cv = specific heats at constant volume and pressure respectively.

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ξ = The factor considering the influence of the lattice optical vibrations on the heat conductivity

The Lattice energy U, molecular weight M, density d, mean acoustic velocity v_m and lattice constant a for alkali halides [3,4] are shown in Table 1. Using eqs. 1–4, thermophysical properties have been evaluated and are shown in Table 2. The experimental values [5] are also given in Table 2 for comparison. One may obtain the following conclusions :

Table 1. Basic data of lattice energy (KJ moles^{-1}), molecular weight, density (Kg-m^{-1}), mean acoustic velocity (ms^{-1}) and lattice constant (A°) for alkali halides.

Alkali Halides	U	M			
LiF	1032	25.94	2601.0	4784.43	4.018
LiCl	851	42.48	2075.3	3396.34	5.140
LiBr	813	86.85	3467.8	2288.27	5.490
LiI	755	133.85	4067.4	1787.51	6.000
NaF	919	41.987	2796.0	3696.13	4.634
NaCl	783	58.442	2162.0	2876.07	5.640
NaBr	747	102.89	3202.5	2098.51	5.950
NaI	699	149.90	3644.0	1678.86	6.462
KF	813	58.096	2525.6	2825.99	5.330
KCl	712	74.551	1986.0	2415.08	6.293
KBr	683	119.00	2747.4	1868.87	6.580
KI	643	166.01	3115.2	1520.05	7.052
RbF	778	104.47	3843.4	2015.52	5.630
RbCl	685	120.92	2796.9	1837.43	6.560
RbBr	658	165.37	3350.0	1529.29	6.600
RbI	622	212.38	3551.0	1316.61	7.325
CsF	742	151.903	4627.0	1591.64	6.895
CsCl	669	168.36	3988.0	1760.30	7.100
CsBr	645	212.81	4456.0	1546.26	7.393
CsI	612	259.82	4524.0	1403.73	7.857

(i) The lattice properties, T_m, K and C_p are linearly dependent on $\theta M^{1/2}$.

(ii) The mean acoustic velocity (v_m) is inversely proportional to square root of molecular weight.

(iii) v_m is also linearly dependent on θ.

The linear dependencies of above lattice properties are shown in Table 1 and obey following relations.

$$K = 6\times10^{-5}\theta M^{2} - 0.0757 \tag{5}$$

$$C_p = -0.0012\theta M^{2} + 14.883 \tag{6}$$

$$\frac{U}{M} = 0.0176\theta M^{2} - 28.112 \tag{7}$$

Table 2. Values of Debye temperature (K), molar volume (m^3), heat capacity (Cal/deg/mol), melting temperatures (K) and thermal conductivity (mW/cm/°K) for alkali halides.

	θ	V_m	C_p	T_m			K
				T_{m1}	T_{m2}	T_m	
LiF	704	9.97	9.54	805	1051.2	**842**	–
LiCl	393	20.47	11.74	696.5	873.6	**614**	0.090
			11.47				
LiBr	248	25.04	12.54	697.4	73.6	**547**	0.052
			11.69				
LiI	177	32.91	12.99	682.5	753.6	**450**	0.040
			12.20				
NaF	475	15.02	11.08	814.9	975.9	**988**	0.107
			11.20				**0.105**
NaCl	304	27.03	11.73	727.2	823	**801**	0.070
			12.07				**0.071**
NaBr	209	32.13	12.47	702.8	768.6	**755**	0.047
			12.28				**0.025**
NaI	155	41.14	12.71	685.1	726.3	**651**	0.362
			12.45				
KF	315	23.00	11.99	786.6	788.9	**846**	0.066
			11.72				**0.071**
KCl	230	37.54	12.38	721.5	748.2	**776**	0.054
			12.26				**0.063**
KBr	170	43.31	12.60	704.2	717.7	**730**	0.040
			12.50				**0.038**
KI	130	53.29	12 72	678.9	672.3	**686**	0.030
			12.65				**0.029**
RbF	212	27.18	12.44	758.2	710.3	**775**	0.042
			12.07				
RbCl	166	43.23	12.62	728.6	694.5	**715**	0.037
			12.52				**0.021**
RbBr	133	49.36	12.73	713.2	666.1	**682**	0.030
			12.63				
RbI	107	59.81	12.82	688.6	629.3	**642**	0.024
			12.71				**0.033**
CsF	158	32.83	12.65	744.2	657.9	**682**	–
			12.21				
CsCl	160	43.22	12.36	809.8	884.3	**646**	–
			12.54				
CsBr	137	47.76	12.77	795.3	885.99	**636**	–
			12.65				
CsI	115	57.43	12.60	774.4	865.51	**621**	–
			12.62				

*The experimental values [5] are presented in bold figures.

$$v_m = \frac{255.37}{\sqrt{M}} - 413.94 \tag{8}$$

$$\theta = 0.01614\ v_m \tag{9}$$

$$T_m = 0.1921\theta M^{\bar{2}} + 370.83 \quad (10)$$

One may state that if molecular weight of a lattice is known, one may get the knowledge of various thermophysical properties and these can be computed using the expressions (5)–(10). The present results are in good agreement with the experimental data.

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